

## FY 2022 First Quarter Performance Metric: Demonstrate Computational Feasibility of the Regional Refined Mesh (RRM) in the Antarctic and the Arctic

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#### 1.0 Product Definition

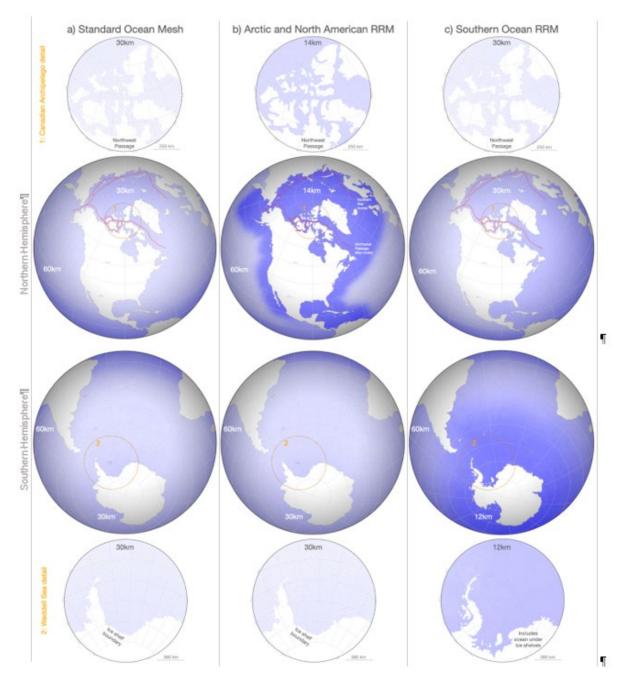
This report summarizes the progress that has been made to configure and generate regionally refined climate simulations in Version 2 of the Energy Exascale Earth System Model (E3SMv2) in a computationally feasible way on Department of Energy supercomputers. E3SM is designed to resolve targeted regions of the globe at high horizontal resolution within a standard-resolution global mesh to improve regional climate reconstructions and projections pertinent to particular science questions. For polar regions, this capability is required to understand feedbacks between global climatic change and regional evolution of the Arctic and Antarctic. More specifically, E3SM has been configured to determine how rapid changes in the cryosphere could evolve with the Earth system and contribute to sea level rise and increased coastal vulnerability. Reductions in the size of the Greenland and Antarctic ice sheets and Southern Ocean ice shelves are anticipated or already underway, and their future mass balance poses the greatest uncertainty in projections of 21st Century sea level rise. It is also important to understand climate feedbacks associated with a diminishing sea ice cover, which extends over 7-10% of the global ocean surface and helps insulate the Earth from solar heating, but has decreased in global extent over the past 40 years.

The capability to refine the Arctic and Antarctic in E3SM rests not just on simulating polar climate using tailored meshes for the ocean, sea ice, atmosphere, and land models in the coupled system, but also on efficient workflows to generate the meshes and configure E3SM to use them. Therefore, we break down the capability into two components. First, we describe the efficiency of the workflow to generate regionally refined meshes (RRMs). This has been greatly improved to reduce the time of configuring RRMs in E3SM from several months to as little as one week. Then, we demonstrate the computational cost of integrating two regionally refined versions of E3SM: one for the Arctic, the other for the Antarctic, relative to the standard-resolution configuration, as well as a global high-resolution configuration.

## 2.0 Product Documentation: Regionally Refined Mesh Generation

#### 2.1 Ocean - Sea Ice

Generating regionally refined ocean-ice meshes for E3SM has become commonplace owing to great advances in the methods used to create unstructured grids for the Model for Prediction Across Scales (MPAS) within which the ocean (MPAS-O) and sea ice (MPAS-SI) are represented as components of E3SM. In this report, we use two illustrative examples of polar ocean sea ice mesh refinement, and compare it to the standard E3SM mesh as illustrated in Figure 1 for Arctic-North American and Southern Ocean refinements, and also to the E3SM globally high-resolution mesh summarized alongside these in Table 1.



**Figure 1.** Comparison of three different meshes available for the ocean and sea ice components as part of E3SMv2. Each column provides four perspectives on each respective grid: (a) the standard E3SM mesh, (b) an Arctic and North American regionally refined mesh (RRM), and (c) a Southern Ocean RRM. Top and bottom rows provide scaled close-ups of (1) the Canadian Archipelago and (2) the Weddell Sea, respectively, illustrating the degree of Arctic and Antarctic refinement relative to one another and the standard mesh in column (a). Amber rings in the broader Northern and Southern Hemisphere perspectives in the second and third rows, respectively, indicate the location of zoomed-in regions of the Canadian Archipelago and Weddell Sea. 12-, 14-, 30-, and 60-km annotations indicate the resolution of the mesh at the given locations on each respective mesh. The Arctic and North American RRM in column (b) refines North American coastal regions as well as the entire Arctic at eddy-permitting ocean scales of 14 km between cell centers, but otherwise has a similar 30-60-km global resolution configuration as the standard

mesh in (a). All configurations resolve key Arctic coastal shipping routes (red), but the Arctic refinement in column (b) ensures the most realistic width of the shipping channels. The Southern Ocean RRM in (c) permits eddies resolved by a 12-km inter-cell grid distance, and represents ocean circulation under Antarctic floating ice shelves.

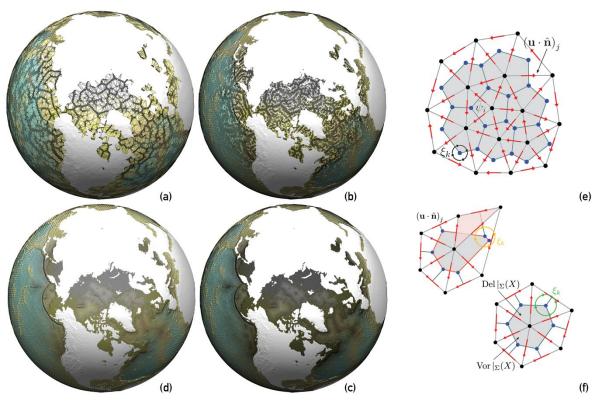
**Table 1.** Summary of component model meshes discussed in this report to resolve regions of interest in E3SM. Ocean meshes are also used by the sea ice model, and the atmospheric mesh resolution applies to land physics and biogeochemistry for the configurations provided in this report. RRM abbreviates Regionally Refined Mesh. Standard and High Resolution provide comparative cases where model resolution is represented relatively evenly around the globe as compared to RRMs. The number of columns indicates the orthographic count of grid points on which scalars such as temperature, atmospheric humidity, ocean salinity, or sea ice thickness are calculated.

	Nominal	Number of Columns
Ocean	Resolution	
C. L. I.B. L.:	20, 601	22 ( 0.52
Standard Resolution	30–60 km	236,853
Arctic and North American RRM	14–60 km	407,420
Southern Ocean RRM	12–60 km	569,915
High Resolution	6–18 km	3,693,225
Atmosphere		
Standard Resolution	110 km	21,600
North American RRM	25-110 km	57,816
Antarctic RRM	25-110 km	48,836
High Resolution	25 km	345,600

The E3SM Version 1 (E3SMv1) mesh generation process for ocean and sea ice components was slow and laborious, requiring several days to generate a standard-resolution mesh and two to three weeks to generate a very high-resolution mesh. Breakthroughs in mesh generation algorithms and the human design interface reduced this generation time by a factor of 50 to 100 in E3SM Version 2 (E3SMv2), down to a few minutes for low resolution and several hours for high-resolution meshes. The mesh-generation algorithm was upgraded from Lloyd's algorithm, which is slow to converge, to the JIGSAW library described below, which achieves significant advances in speed by strategically adding and removing cells in the iterative process. Equally important, a convenient and well-documented interface, COMPASS (https://mpas-dev.github.io/compass), allows modelers to design variable-resolution meshes based on distance from coastlines and shapes drawn with an online tool, with geometric parameters that are easy to adjust on the fly. COMPASS tracks how each mesh was created to ensure long-term reproducibility. In combination, these improvements have led to a much faster turnaround in the mesh design, simulation, and feedback process, so that modelers can consult with domain experts to explore a number of configurations and produce the best simulations for the computational cost. This is the process used to generate the Arctic and Southern Ocean refinements in Figure 1, and has ensured, for example, that all major Arctic shipping pathways are open in E3SMv2. A practical demonstration of the mesh approval process for these respective meshes can be found on GitHub for the Arctic and Antarctic.

Leveraging the JIGSAW unstructured meshing library (Engwirda 2017) has enabled the creation of complex, variable-resolution meshes to resolve regional sea-ice (Turner et al. 2021), ocean (Hoch et al. 2020), and land-ice (Hoffman et al. 2018) dynamics. Compared to the initial *optimization-only* meshing approaches pursued in E3SMv1 (Jacobsen et al. 2013), the unstructured meshing kernels in the JIGSAW library take a number of alternative pathways to solving the various computational-geometric and algorithmic problems inherent to the generation of the spherical Centroidal Voronoi Tessellations (CVTs) (Ringler et al. 2008) used in the MPAS-O and MPAS-SI dynamical cores.

• Efficient initialization: The creation of optimal CVT meshes is known to be a difficult optimization problem (Du et al. 1999), requiring a potentially very large number of expensive global iterations to converge toward a high-quality mesh given an arbitrary initial distribution of points and cells. In the JIGSAW library, a multi-paradigm meshing strategy is used — first building an initial mesh based on a so-called *off-center* Delaunay-refinement scheme (Engwirda and Ivers 2016) to provide a high-quality initial condition for the subsequent CVT mesh optimization passes. As per Figure 2 (a-d), this fractal-like approach generates initial meshes that are already largely quasi-optimized, significantly reducing the burden on the final, computationally expensive, mesh optimization procedure.



**Figure 2.** Details of the E3SMv2 mesh generation workflow, showing: (a)-(d) the generation of quasi-optimal mesh initial conditions for an example of regionally refined configuration, based on JIGSAW's off-center Delaunay-refinement approach, (e) an example of a well-conditioned staggered polygonal-triangular CVT mesh, with all edges, triangles, and polygons oriented optimally with respect to one another, and (f) an example of a poorly-staggered mesh configuration (upper subfigure), in which paired edges (highlighted) in adjacent polygons and (obtuse) triangles do not intersect, leading to a breakdown in the MPAS numerical discretization. This may be rectified, as illustrated in the lower subfigure of (f).

- Coupled geometry and topology optimization: The construction of optimal CVT meshes is a coupled optimization problem requiring both a high-quality arrangement of mesh vertices (geometry) as well as optimal connectivity between mesh cells (topology). In the JIGSAW library, an expanded set of mesh optimization predicates is introduced (cell collapse, progressive refinement), as well as a nonlinear *hill-climbing* optimization schedule that focuses on improving the worst-quality cells in a mesh at each CVT iteration (Engwirda 2017, 2018). These methods improve the quality and robustness of the E3SMv2 meshing workflow, ensuring that the resulting polygonal-triangular meshes (see Figure 2e) are well conditioned with respect to MPAS-type numerical methods. A key difficulty associated with the E3SMv1 meshing approach was the generation of invalid staggered grid configurations (see Figure 1f) in which adjacent polygonal and triangular cells were not consistently staggered with respect to one another. These poor-quality grid configurations lead to a breakdown in the MPAS discretization, and thus limited the use of varying mesh resolution in E3SMv1. This lack of robustness has been remedied in E3SMv2, with JIGSAW's enhanced mesh optimization strategies leading to valid, well-conditioned, staggered meshes in complex, regionally refined cases.
- Minimal algorithmic complexity: Significant computational efficiency can be gained by exploiting advanced data-structures and algorithmic constructs to reduce the expense of operations on large-scale meshes. The JIGSAW library is structured around efficient, local updates to global mesh data-structures, leading to a quasi-optimal O(nlog(n)) implementation. An approach based on linear, global data-structures was taken in the original E3SMv1 meshing algorithm, requiring a much-expanded O(n³) overall operations count. Noting the large size of meshes for E3SM (e.g., n >= 1 x 10⁵), the reduction of algorithmic complexity from O(n³) to O(nlog(n)) represents an orders-of-magnitude improvement in runtime.

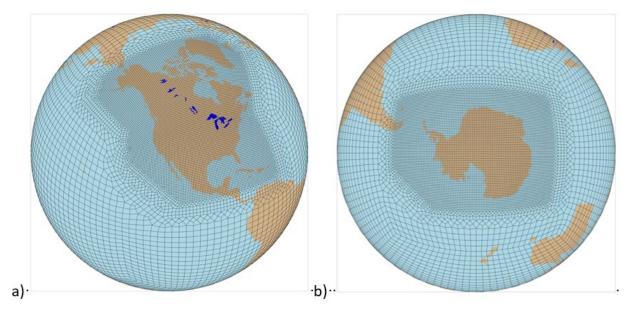
Taken together, these improvements to the E3SMv2 meshing kernels represent a significant expansion to the regional-refinement capabilities available for the MPAS-O and -SI dynamical cores, enabling simulations incorporating complex patterns of regional, variable resolution to resolve fine-scale dynamics of interest, as illustrated for the Arctic and Antarctic in Figure 1.

#### 2.2 Atmosphere - Land

The E3SM Atmosphere Model (EAM) adopts a highly scalable spectral element dynamical core that supports variable resolution through regional mesh refinement (Dennis et al. 2012, Guba et al. 2014, Taylor 2021). The Regionally Refined Mesh (RRM) capability in EAM preserves its key conservation and scalability features and has been demonstrated to improve simulations over refined regions comparable to globally uniform high resolution without negatively impacting the performance elsewhere (Rasch et al. 2019, Tang et al. 2019, Zarzycki et al. 2015). As an example, the Antarctic mesh in Figure 3 enhances resolution over the Southern Ocean while also improving the representation of complex terrain on the Antarctic continent. It is designed to improve simulations of consequential synoptic-to-local-scale phenomena, including meso-scale structure along Southern Hemisphere storm tracks and katabatic winds over coastal Antarctica.

The meshes in Figure 3 have uniform 25-km resolution within the refined area and gradually transition to EAM's standard resolution of 110 km elsewhere. The established workflow, documented on the E3SM Confluence space, is used to create the mesh (based on Taylor and Zarzycki 2014) and generate the supporting files (Hillman et al. 2021) for simulations with E3SM. The RRM was generated using the Spherical Quadrilateral Mesh Generator (SQuadGen, Ullrich 2015), following a procedure developed by

Guba (2014), which is the preferred approach for mesh refinement over an unstructured area (i.e., with non-functional-form periphery). SQuadGen uses a specified PNG image in grayscale to define the refinement area, with the level of refinement determined by shading, which can be either from white to black or the other way around. The transition zone can thus be controlled via gradient shading. The user-specified PNG image typically uses the standard-resolution (110 km, Table 1) global mesh in equidistant cylindrical projection as the background to aid the placement (or "drawing") of the region of interest for refinement. This can be done using an image editor (e.g., Photoshop, GIMP). The PNG image saved from the overlaid drawing will be the image to feed SQuadGen to generate the RRM mesh in exodus format. The refinement level is specified as a command-line option to SQuadGen. The generated mesh is visually inspected using grid-plotting utilities, refined through further editing of the specified PNG file as needed, and iterating on this process until arriving at a final satisfactory mesh.



**Figure 3.** Refinement of the atmospheric mesh for (a) North America including the American Arctic and (b) the Antarctic-focused simulations in E3SM, with resolution ranging between 25 km and 110 km outside of detailed areas. Cell counts for the displayed meshes are provided in Table 1.

The new grid can be tested by running an idealized baroclinic instability problem (Jablonowski and Williamson 2007) in HOMME (the spectral element dynamical core) standalone mode (following Taylor and Zarzycki 2014). The quality of the RRM can also be examined in terms of the degree of element distortion computed when running HOMME in E3SM or standalone. Ultimately, the RRM mesh needs to be tested in the full EAM or E3SM. To run the full model with the RRM mesh, supporting files are required to define the dynamical structure, initialize the atmosphere model, and enable the coupling of the atmospheric RRM with the other E3SM components. These include the initial condition files, the topography file, the mapping and domain files, and the corresponding control volume mesh file that is used in E3SMv2 with physics grid (pg2). The full procedure is documented in the step-by-step guide for running E3SM on a new grid (Hillman et al. 2021). The dynamical core parameters for running the RRM are typically set to be the same as required by the finest grid in the RRM. The model physics step in E3SMv2, however, is set to be the same as required by the base grid (i.e., 110-km-resolution grid for this Antarctic RRM). This choice benefits the simulation throughput and minimizes the need for tuning, as the standard model has been well tuned and any retuning for the interest of the refined region could have

global implications. With these parameter settings, the EAM running on this Antarctic RRM is 2.5 times as expensive as the standard model, only slight larger than the ratio of the number of spectral elements between the two meshes.

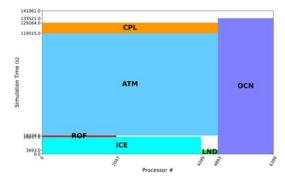
# 3.0 Results: Arctic and Antarctic Regionally Refined Coupled Simulations in E3SM

To demonstrate the computational feasibility of simulating global climate in E3SM using regional refinement in either the Arctic or the Antarctic, we present run-time statistics for four fully coupled configurations of the model. By fully coupled, we mean that all of the atmosphere, ocean, sea ice, and land components of the model dynamically exchange energy and mass (e.g., heat and water) with other parts of the system as occurs in the natural Earth system. The E3SM atmospheric model (EAM), land model (ELM), land hydrology (MOSART), ocean model (MPAS-O), and sea ice model (MPAS-SI) are all active in the cases we present, colloquially referred to as B-case simulations. These components can be configured to use any combination of a regionally refined ocean-sea ice mesh with the standard-resolution atmosphere-land grid in Table 1, or vice versa. E3SM can also use a regionally enhanced mesh for both ocean-sea ice and atmosphere-land components.

To illustrate the versatility of mixing different component mesh configurations, we present timing statistics for two regionally refined configurations summarized in Table 2, and compare these with the standard and globally high-resolution E3SM configurations. One regionally refined simulation is for the Arctic, the other for the Southern Ocean, which make respective use of ocean meshes shown in columns (b) and (c) of Figure 1. The Arctic refinement also uses the North American atmospheric mesh in Figure 3a, of which roughly half of the refinement covers the American portion of the Arctic System, as defined by Roberts et al. (2011). The Southern Ocean refinement uses a standard atmospheric mesh without atmosphere-land resolution enhancement. For the purpose of this report, we focus on load-balanced configurations specific to a recently acquired high-performance Department of Energy computer, Chrysalis, which is an AMD machine with 512 nodes and 64 cores per node. Load balancing requires that component models of E3SM be allocated a specific number of cores within the total core count in Table 2 to minimize wasted computing time across the parallel architecture. An example of load balancing is provided in Figure 4 for the Refined Arctic and North America configuration.

**Table 2.** Comparison of the computational cost of two regionally refined configurations of E3SMv2 for the Arctic and Antarctic optimized for the Department of Energy AMD computer Chrysalis (512 nodes, dual socket, 64 cores per node, "Rome" processors), compared with the standard, lower-resolution version of E3SM, and the global high-resolution configuration. The core count indicates the total number of cores used to integrate the model, the core hours indicate the total computational cost to execute a one-year integration of E3SM in that configuration, and the throughput indicates how many years the model can simulate each day in these configurations. Throughput of the high-resolution configuration appears in parenthesis because this particular test case could use a much higher core count to increase that number if desired. RRM names and column counts are provided in Table 1.

E3SM Configuration	Atmosphere–Land Mesh	Ocean–Sea Ice Mesh	Chrysalis Core count	Core hours per simulated year	Throughput in simulated years per day
Standard	110 km globally	30-60 km globally	6784	3115	26.13
Refined Arctic and North America	North American RRM	Arctic and North American RRM	12800	12539 (~4 x)	12.25
Refined Southern Ocean	110 km globally	Southern Ocean RRM	13440	8842 (~3 x)	18.24
High Resolution	25 km globally	6-18 km globally	8192	107901 (~35 x)	(0.91)



**Figure 4.** Load balancing of E3SM for the Refined Arctic and North America configuration in Table 2 on the Department of Energy AMD computer Chrysalis, where the total area of each block indicates the total time spent in executing each part of the model. Legend: ICE-sea ice model (MPAS-SI), LND-land model (ELM), ROF-land runoff (MOSART), ATM-atmospheric model (EAM), OCN-oceanic model (MPAS-O), CPL-coupling and model infrastructure. The relative lack of white space indicates that the model is making efficient use of the available nodes during execution of this regionally refined configuration.

The most important results of this report are presented in Table 2 in the total core hours per simulated year of the model, and the computational throughput. First, compare the throughput in Table 2 (bold numbers), which is the number of years simulated by E3SM each day. These illustrate that regional Arctic atmospheric, land, ocean, and sea ice refinement can achieve about 46% of the throughput as the standard model at between twice and a little more than four times the standard resolution for the American Arctic, as well as the broader Arctic Ocean. If one is only to refine the marine component for Antarctic and Southern Ocean investigations, but more than double the total number of ocean grid cells, a throughput of nearly 70% of the standard model is achieved at around three times the computational cost (core hours per

simulated year). As a consequence, regional refinement presents an attractive alternative to simulating global climatic feedbacks and impacts in polar regions in E3SM when global high resolution is deemed too expensive. We note that many more cores could have been allocated to the E3SMv2 high-resolution case in Table 2 to improve throughput, but the total core hours would be less sensitive to that change and would be significantly more than for the RRM configurations in Table 2. For the Arctic refined case presented here, a 1,000-year pre-industrial climate spin-up would take a little over 80 days to execute. This translates to about 70 days to sequentially generate five ensemble members to reconstruct the E3SM climate of the industrial era starting in 1850. For the Southern Ocean configuration, the corresponding experiment lengths are 55 and 47 days, respectively, making regional refinement in E3SM computationally tractable to analyze regional polar climate change.

These results indicate that it is not only feasible to refine the Arctic or Antarctic in E3SM to address polar science questions, but computationally desirable, with high efficiency compared to global high resolution, and with comparable efficiency to standard resolution. By extension, E3SM mesh refinement elsewhere on the globe is also feasible and could often be the tool of choice to address science questions applicable to lower-latitude regions using fully coupled integrations spanning 1,000 years or more.

### 4.0 Contributors to this Report

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